1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{26}\text{H}_{29}\text{Cl}_{2}\text{N}_{5}\text{O}_{3} \cdot 0.5\text{H}_{2}\text{O} \)

Batch Molecular Weight: 539.46

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:

![Molecular Structure](image)

2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

\(^1\text{H NMR:}\) Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>57.89</td>
<td>57.72</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.61</td>
<td>5.81</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>12.98</td>
<td>12.95</td>
</tr>
</tbody>
</table>
Product Name: Bosutinib
Catalog No.: 4361
Batch No.: 1

CAS Number: 380843-75-4
IUPAC Name: 4-[(2,4-Dichloro-5-methoxyphenyl)amino]-6-methoxy-7-[3-(4-methyl-1-piperazinyl)propoxy]-3-quinolinecarbonitrile

Description:
Dual inhibitor of Abl and Src kinases (IC_{50} = 1.2 nM for Src in an enzymatic assay). Displays antiproliferative activity against chronic myelogenous leukemia (CML) cells and decreases the motility and invasion of breast cancer cell lines. Also exhibits potent antiproliferative activity in anchorage-independent, Src-transformed rat fibroblasts (IC_{50} = 100 nM). Displays selectivity for Src over non-Src family kinases such as growth factor receptor tyrosine kinases.

Physical and Chemical Properties:
Batch Molecular Formula: C_{38}H_{30}Cl_{2}N_{5}O_{3}½H_{2}O
Batch Molecular Weight: 539.46
Physical Appearance: Pale yellow solid
Minimum Purity: >99%

Storage: Store at +4°C

Solubility & Usage Info:
Soluble to 100 mM in DMSO and to 25 mM in ethanol

Stability and Solubility Advice:
Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:
SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.
SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Congratulations on your purchase of Bosutinib, sold under license from Pfizer, Inc. If your research with Bosutinib results in an new discovery (e.g., new uses, new combinations, etc.) Pfizer is interested in discussing these discoveries with you. Also note that Pfizer has a Compound Transfer Program that provides a free sample of any Pfizer product at www.pfizer.com/research/rd_works/compound_transfer_program.jsp

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use